Russian Journal of General Chemistry 1998 vol.68 N11, pages 1837-1840

Electronic and Steric Structure of Tricarbonyl(5-pheny--1,3-dioxane)chromium

Filatov M., Aminova R., Aganov A.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

According to the results of quantum-chemical calculations, the conformation of 5-phenyl-1-3-dioxane changes upon complex formation with tricarbonylchromium. The most favorable conformation in the complex is chair with the axial phenyl group oriented along the symmetry plane of the dioxane ring. The tricarbonylchromium fragment is located above the benzene ring plane. The calculated spin-spin coupling constants suggest presence in solution of a mixture of conformers, that with the axial substituent prevailing.